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Predicting the compositional evolution of the structure and properties of oxide glasses is important for designing new materials for advanced applications. In aluminoborate glasses, the structural role of aluminum highly depends on the modifier concentration. When the modifier oxide concentration exceeds that of alumina, aluminum is primarily found in a 4-fold coordinated network-forming site. At lower relative modifier concentration, aluminum becomes 5- or 6-fold coordinated. The bonding preference of these high-coordinated aluminum ions have not yet been fully understood. In this study, we develop a statistical mechanics model to describe the composition-structure relation in the ternary Na_2O-Al_2O_3-B_2O_3 glass system. We find that the structure of Cs_2O-Al_2O_3-B_2O_3 and Li_2O-Al_2O_3-B_2O_3 glasses can be accurately described using the Al-B interaction parameters determined for the Na_2O-Al_2O_3-B_2O_3 glasses. Our findings thus give new insights into the bonding preferences for both high-coordinated aluminum species and alkali cations.

Reference: Bødker M. S., Christensen R., Sørensen L. G., Østergaard M. B., Youngman R. E., Mauro J. C., Smedskjaer M. M. Predicting Cation Interactions in Alkali Aluminoborate Glasses using Statistical Mechanics. *Journal of Non-Crystalline Solids* **544**, 120099 (2020).